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Event-by-Event Fission Modeling with FREYA (U)

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Current radiation transport codes compute average quantities with great accuracy and performance but performance and averaging comes at the price of limited interaction-by-interaction modeling. For fission applications these codes often lack the capability of modeling interactions exactly: energy is not conserved; energies of emitted particles are uncorrelated; and prompt fission neutron and photon multiplicities are uncorrelated. Many modern applications require more exclusive quantities than averages, such as the fluctuations in certain observables (e.g. the neutron multiplicity) and correlations between neutrons and photons. The fast event-by-event fission code FREYA generates large samples of complete fission events. Using FREYA, it is possible to obtain the fission products as well as the prompt neutrons and photons emitted during each individual fission process, all with complete kinematic information. We can therefore extract any desired correlation observables. Concentrating on ^{239}Pu(n,f), ^{235}U(n,f) and ^{252}Cf(sf), we compare our FREYA results with available data on prompt neutron and photon emission. FREYA has been integrated into the LLNL fission library, an integral part of MCNP6. By comparing Monte Carlo simulations performed with and without FREYA, we have found that the fluctuations and correlations introduced lead to significant differences that can be measured experimentally. (Unclassified)

Introduction to FREYA

This contribution describes recent results with the FREYA (Fission Reaction Event Yield Algorithm) code being developed at LLNL in collaboration with LBNL. FREYA is unique in that it is a fast fission simulation that treats fission on an event-by-event basis. Here we first describe the basic physics of FREYA. We then describe how it differs from other available models. Finally, we show some of the results achieved when FREYA is included in the MCNP transport code, a major aim of the project.

FREYA is designed to simulate binary fission. The fissioning system is either a compound nucleus created by absorption of a neutron (or a photon) by a fissile nucleus such as ^{239}Pu or ^{235}U or a nucleus that undergoes spontaneous fission, such as ^{252}Cf. The initial nucleus may have a finite angular momentum. For neutron-induced fission, the angular momentum is imparted to the system by the incident neutron.

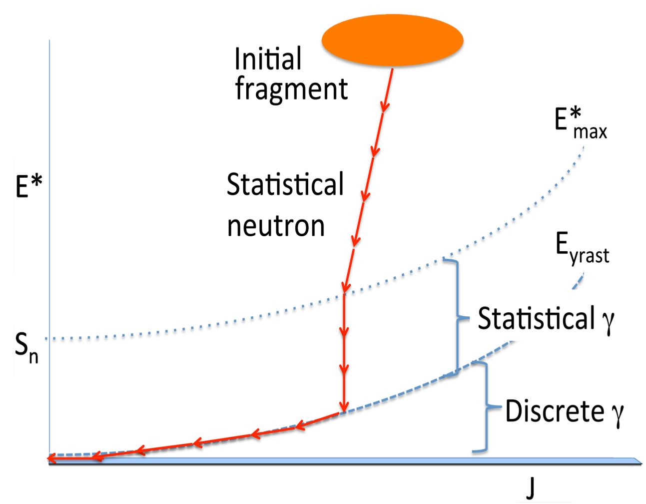

Fig. 1. Schematic depiction of the sequential de-excitation of a hot fission fragment by: first prompt neutron evaporation; then statistical photon emission; and finally photon emission along the yrast line down to the ground state.

Neutron emission prior to fission is also allowed in the case of neutron-induced fission. We account for pre-equilibrium emission where the compound nucleus does not form but the incident neutron is re-emitted. In this case, some of the energy imparted to the system by the incident neutron remains in the system and can cause fission after the neutron is emitted. The fissioning nucleus is thus ^{239}Pu* rather than ^{240}Pu*, as is the case when the neutron is not emitted. We also include multi-chance fission. In this case, the compound nucleus is formed and loses some of its excitation energy by evaporating neutrons before ultimately fissioning. If the initial compound nucleus fissions, this is known as first-chance fission. If one neutron is emitted prior to fission, we have second-chance fission, and so on. Pre-equilibrium emission and multi-chance fission grow increasingly important at higher incident neutron energies. They are negligible at thermal neutron energies but are significant for 14 MeV neutrons. They play no role in spontaneous fission.

When fission occurs, the identities of the fission fragments are determined by sampling from mass and charge distributions, based on either models or data. Once the mass and charge of a single fragment has been sampled, those of the partner fragment follow from mass and charge conservation.

Once we have identified the mass A and charge Z of the light and heavy fragments, we can calculate the fission Q value. The Q value has contributions from the fragment kinetic energies, internal excitation energies and rotational energy, imparted to the fragments at scission. We sample the rotational energy from the rotation of the fissioning system as a whole (rigid rotation around a common axis) and also allow for relative angular momentum of the two fragments in the bending and twisting modes (where they rotate in the same or opposite directions relative to each other). The total kinetic energy of the fragments, TKE, is sampled from measured distributions. The total intrinsic excitation energy, TXE, is found by subtracting TKE and the rotational energies from the Q value. We allow for statistical fluctuations in the fragment excitation energies, making corresponding adjustments in TKE to conserve total energy.

Neutron evaporation from the fully accelerated fragments conserves energy as well as linear and angular momentum at each step. It continues until the residual excitation energy is below the neutron separation energy, i.e. too low for further neutron emission. We allow for statistical photon emission down to the yrast line from where photon emission follows stretched E2 transitions until the spin is depleted (Fig. 1). FREYA provides the full kinematic information on the two fission product nuclei and all of the emitted neutrons and photons.

There are several adjustable parameters in FREYA. The asymptotic level density parameter, important for setting the temperature scales and thus the excitation energies all through the fission process, is assumed to be the same for all fissioning nuclei. It was set in our evaluation of ^{239}Pu(n,f)[1]. We also have a parameter that allows a shift in the excitation energy balance between the light and heavy fragments, giving some extra energy to the light fragment since it emits more neutrons on average than the heavy fragment. For ^{239}Pu(n,f) this parameter is 1.1, for ^{252}Cf(sf), it is 1.3. The overall magnitude of the TKE is adjusted to match the measured value of the average neutron multiplicity. This shift is typically on the order of 0-2 MeV and may exhibit some energy dependence for neutron-induced fission. (It is almost independent of energy for ^{239}Pu(n,f) but rises with incident neutron energy for ^{235}U(n,f).) Finally, we can adjust the rotational energy through a 'spin temperature', proportional to the temperature of the system at scission. This parameter has little to no effect on neutron observables, as long as the average neutron multiplicity is unchanged, but has a strong effect on the photon observables.

FREYA was developed as a standalone code and various analysis routines have been written to extract various observables, including neutron multiplicities as a function of fragment mass, prompt fission neutron spectra for different neutron multiplicities, neutron-neutron correlations and neutron-photon multiplicity correlations.[1,2,3,4,5] It has been released as an open source code available for public use and a user manual is currently being written for the released version. We expect that it will also become part of the MCNP6 release within the next couple of year, implemented as a callable fission routine and allowing the user to extract any observable of interest. The LLNL fission library[6], which samples the ejectiles independently, without taking account of any prior emissions, has been augmented to include FREYA.

Comparison of Fission Models

Table 1 below compares how MCNP/MCNPX and GEANT treat neutron and photon emission in fission events relative to a version of MCNP with FREYA incorporated in it. The process is illustrated schematically for MCNPX and FREYA in Fig. 2.

Table 1. The performance of several different available transport codes for prompt neutron and photon emission during fission events are compared.

Code	#n/fission	#γ/fission
MCNP/X[7]	Analog	Based on total cross section, not analog
GEANT[8]	Limited isotopes, analog	Single isotope, analog
MCNP+FREYA	Analog	Analog

The default in MCNP/MCNPX heretofore has been to first emit photons without the code identifying which reaction took place. Thus the photons emitted were uncorrelated with the reaction but were instead taken from all possible reactions that could produce photons. Only after photon emission was the type of neutron-induced reaction chosen. Thus, as stated in Table 1, the photon multiplicity is based on the total cross section and is not an analog process (which assumes prior knowledge of the past event). Neutron emission follows once the reaction has been identified as being a fission event and is thus analog. In GEANT, both neutron and photon emission are analog. However, the number of available isotopes is limited and, in the case of photons, only one isotope is used for all fission photons. FREYA treats both neutron and photon emission as analog (all retained FREYA events are fission events) and the emissions are unique to the fissioning nucleus, not based on a common, average, distribution. However, to make FREYA fully functional in MCNP6, the way that photons are handled in MCNP6 must be modified to accommodate the more complex event information provided by FREYA.

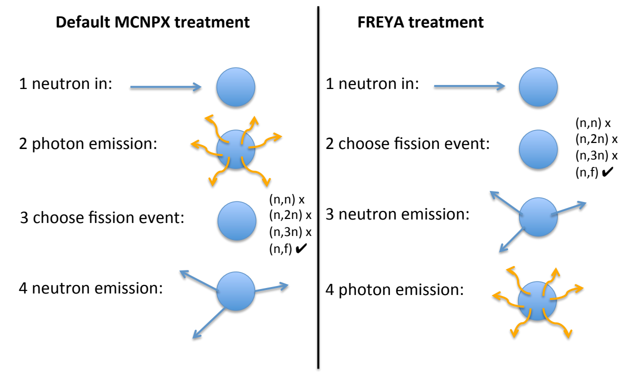

Fig. 2. FREYA (right) compared to the MCNPX (left) treatment of fission.

Relevant Results

The results shown in this section were obtained by embedding FREYA into a version of MCNP5 (Fig. 3, simulated by C. Hagmann[9]) and a version of MCNPX with FREYA incorporated into the LLNL fission library (Figs. 4 and 5, simulated by M. James[10]).

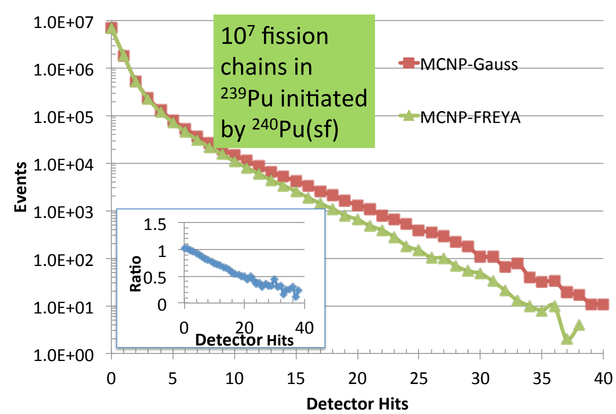

Fig. 3. Simulation of 10^7 fission chains with M=6 in ^{239}Pu initiated by ^{240}Pu(sf)[9] with MCNP+Gauss multiplicity distribution and MCNP+FREYA. The inset shows the ratio of MCNP+FREYA to MCNP+Gauss as a function of number of detector hits.

The results shown in Fig. 3[9] were obtained by adopting the MCNP detector model developed for a large array of liquid scintillators[11,12]. The detector consists of 64 xylene cells, each read out by a single phototube. The cells are symmetrically arranged into octants with an inner diameter of 60 cm. The detector was designed for fast multiplicity counting. Neutron-photon separation is accomplished by pulse-shape discrimination with a minimum proton recoil energy of ~1 MeV and a corresponding detection efficiency of ~ 5%.

A ^{240}Pu(sf) source was placed at the center of the array. To study neutron multiplication greater than unity, chains in a Pu ball (94% ^{239}Pu, 6% ^{240}Pu) were initiated by ^{240}Pu(sf). Runs with the MCNP+Gauss (Gaussian neutron multiplicity distribution) setup used the MCNP Watt fission parameters for ^{240}Pu(sf) and an isotropic neutron emission angle. All neutron data for ^{239}Pu came from ENDF/B-VII.0 except when sampling fission events with MCNP+FREYA[9]. FREYA predicts a progressively softer neutron energy spectrum with increasing neutron multiplicity, reflecting the decreasing fragment excitation energy as successive neutrons are evaporated. In contrast, MCNP+Gauss samples all neutrons from a common, 'average' spectrum.

Figure 3 shows the calculated detector multiplicity distributions for a multiplying Pu ball with M=6. There are 10^7 source events. A detector cell was triggered if one or more proton recoils with energy greater than 1 MeV occurred in the same Monte Carlo history. MCNP+FREYA predicts a smaller number of events at large multiplicities than MCNP+Gauss. The inset shows the ratio of the two distributions. It is clear that the softening of the spectrum in FREYA makes a significant difference in the two results.

We now turn to neutron-neutron angular correlations. Most neutrons in low energy neutron-induced fission are emitted by fully accelerated fragments moving apart back-to-back in the laboratory frame. FREYA emits neutrons isotropically in the moving rest frame of the fragments and boosts them back into the laboratory frame. Thus, in the laboratory frame, the neutrons exhibit kinematic clustering around the fragments, resulting in angular correlations. If one neutron is emitted from each fragment, the relative angle is peaked at 180°. On the other hand, the n-n angular correlation is peaked at 0° if both neutrons are emitted from one of the two fragments. The correlation is stronger if both neutrons come from the light fragment since it has a higher velocity.

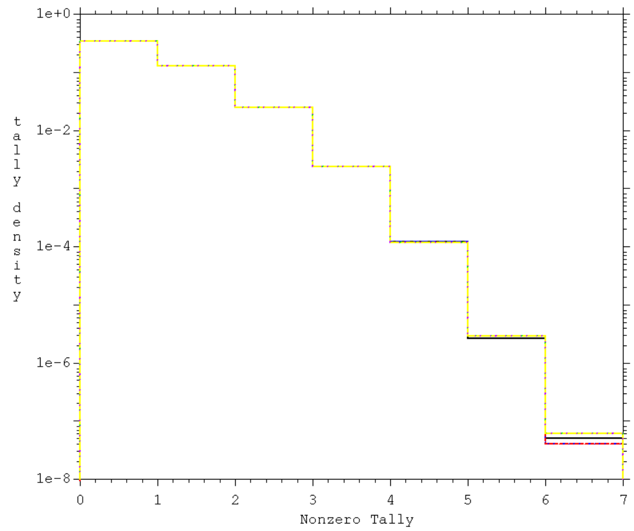

Fig. 4. Tallies of neutron hits on opposite and adjacent faces of a cube with a ^{235}U neutron source inside, obtained from MCNPX simulations employing the LLNL fission library[10].

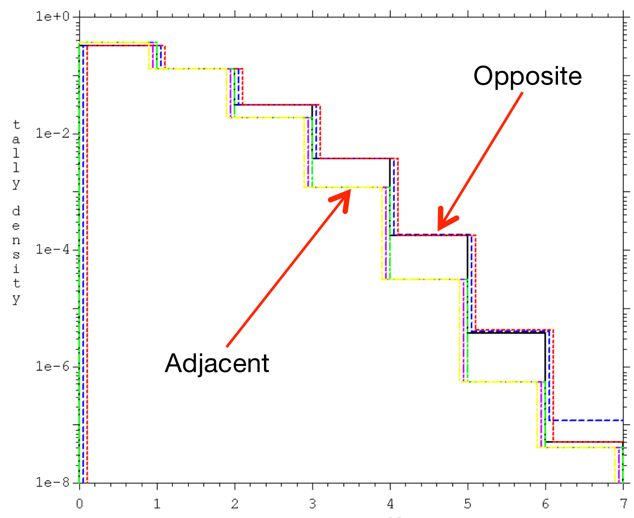

Fig. 5. Same as Fig. 4 but now the simulations employ the LLNL fission library with the event-by-event code FREYA[10]. The x-axes offsets are for clarity.

Figures 4 and 5 show test runs of our released version of FREYA, embedded in the LLNL fission library and in MCNPX. The results were obtained by M. James of LANL[10]. In these simple test simulations, a ^{235}U source was placed inside a cube. Tallies were made on opposite and adjacent cube faces. If neutron emissions are correlated according to FREYA, the opposite faces should have higher tallies than the adjacent faces. In Fig. 4, the results are shown for the LLNL fission library alone. This library has only uncorrelated neutron emission so that the opposite and adjacent tallies are identical. On the other hand, the results with FREYA show a clear correlation with a higher tally density for hits on opposite faces than for adjacent faces.

Summary

Event-by-event modeling of fission in FREYA shows significant directional correlations between neutrons evaporated from the fragments. These correlations have recently been observed in experiments[13]. The first version of FREYA has been released to the public and will be made available in MCNP6.

Acknowledgments

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